Thermodynamic potentials from shifted boundary conditions

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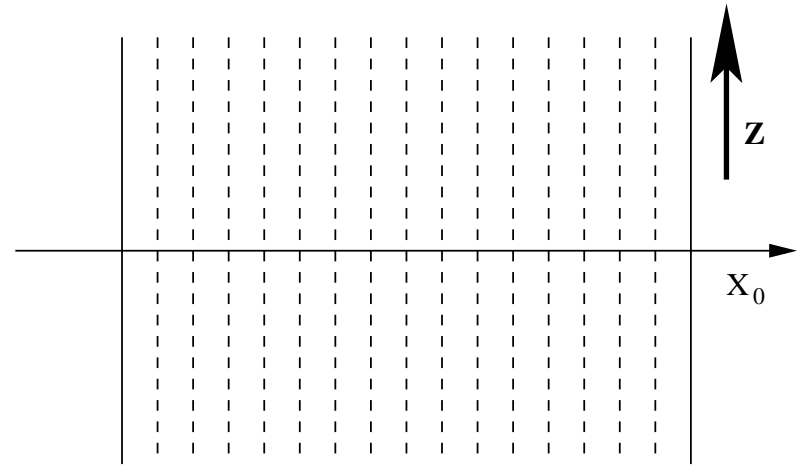
Outline

- Relation between the entropy density and the response of the system to the shift

$$s = -\frac{1}{T^2} \lim_{V \to \infty} \frac{1}{V} \frac{d^2}{dz^2} \ln Z(\{0,0,z\})\Big|_{z=0}$$

- Generalization to the specific heat

- Finite-size effects

- Extension to the lattice (and exploratory numerical study for $SU(3)$ Yang–Mills)
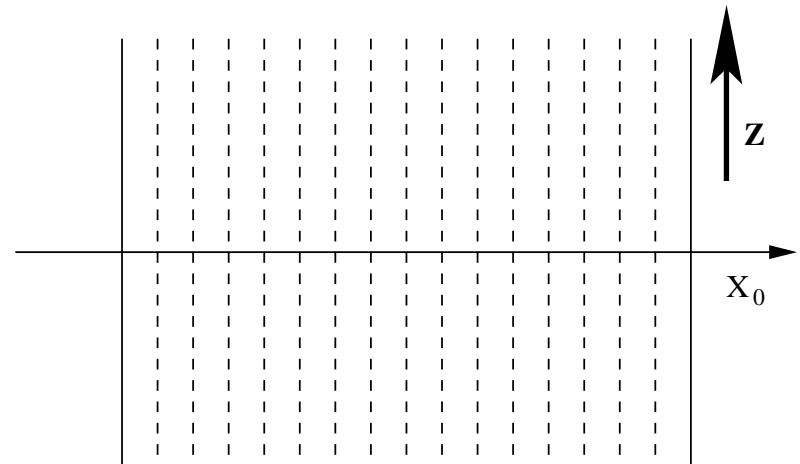
- Conclusions and outlook

Momentum distribution from shifted boundary conditions

- The relative contribution to the partition function of states with momentum $\mathbf{p}$ is $[T = 1/L_0]$

$$\frac{R(\mathbf{p})}{V} = \frac{\mathrm{Tr}\{e^{-L_0\hat{\mathrm{H}}}\,\hat{\mathrm{P}}(\mathbf{p})\}}{\mathrm{Tr}\{e^{-L_0\hat{\mathrm{H}}}\}}$$

where

$$\hat{\mathrm{P}}(\mathbf{p}) = \frac{1}{V}\int d^3\mathbf{z}\,e^{-i\mathbf{p}\cdot\mathbf{z}}\,e^{i\hat{\mathbf{p}}\cdot\mathbf{z}}\ , \qquad e^{i\hat{\mathbf{p}}\mathbf{z}}|\phi\rangle = |\phi^{\mathbf{z}}\rangle$$

- The momentum distribution can then be written as

$$\frac{R(\mathbf{p})}{V} = \frac{1}{V}\int d^3\mathbf{z}\,e^{-i\mathbf{p}\cdot\mathbf{z}}\,\frac{Z(\mathbf{z})}{Z}\ , \qquad \phi(L_0,\mathbf{x}) = \phi(0,\mathbf{x}+\mathbf{z})$$

where $Z(\mathbf{z})$ is the usual path integral but with shifted boundary conditions in time direction

Cumulant generator

● As usual the generator of its cumulants is defined as

$$
e^{-K(\mathbf{z})} = \frac{1}{V} \sum_{\mathbf{p}} e^{i\mathbf{p}\cdot z} R(\mathbf{p}) \qquad \Longrightarrow \qquad e^{-K(\mathbf{z})} = \frac{Z(\mathbf{z})}{Z}
$$

● The momentum cumulants can then be written as

$$
\frac{\langle \hat{p}_1^{2n_1} \, \hat{p}_2^{2n_2} \, \hat{p}_3^{2n_3} \rangle_c}{V} = \frac{(-1)^{n_1+n_2+n_3}}{V} \frac{\partial^{2n_1}}{\partial z_1^{2n_1}} \frac{\partial^{2n_2}}{\partial z_2^{2n_2}} \frac{\partial^{2n_3}}{\partial z_3^{2n_3}} \ln\left[\frac{Z(\mathbf{z})}{Z}\right]_{\mathbf{z}=\mathbf{0}}
$$

● In the continuum they equal the standard definition

$$
\langle \hat{p}^{2n_1} \, \hat{p}^{2n_2} \, \hat{p}^{2n_3} \rangle_c = (-1)^{n_1+n_2+n_3} \langle \overline{T}_{01} \cdots \overline{T}_{03} \rangle_c \, , \qquad \overline{T}_{0k}(x_0) = \int d^3x \, T_{0k}(x)
$$

and, being conn. corr. functions of the momentum charge, they are finite as they stand. The generator $K(\mathbf{z})$ and the distribution $R(\mathbf{p})$ are thus expected to be finite as well

Momentum distribution from shifted boundaries on the lattice [Della Morte, LG 10; LG, Meyer 10]

- On the lattice a theory is invariant under a discrete group of translations only. It is still possible, however, to factorize the Hilbert space in sectors with definite conserved total momentum

- The momentum distribution is given by

$$\frac{\mathcal{R}(\mathbf{p})}{V} = \frac{a^3}{V} \sum_{\mathbf{z}} e^{-i\mathbf{p}\cdot\mathbf{z}} \frac{\mathcal{Z}(\mathbf{z})}{\mathcal{Z}}$$

where $\mathcal{Z}(\mathbf{z})$ is the usual PI but with (discrete) shifted boundary conditions.

- Since only physical states contribuite to it, $\mathcal{R}(\mathbf{p})$ is expected to converge to the continuum universal value without need for UV renormalization

- The shifted boundary conditions allow us to define connected correlation functions of the momentum which do not require any UV renormalization

- Their continuum limit satisfies the standard EMT WIs, which can be used to interpret the cumulants in terms of basic thermodynamic potentials
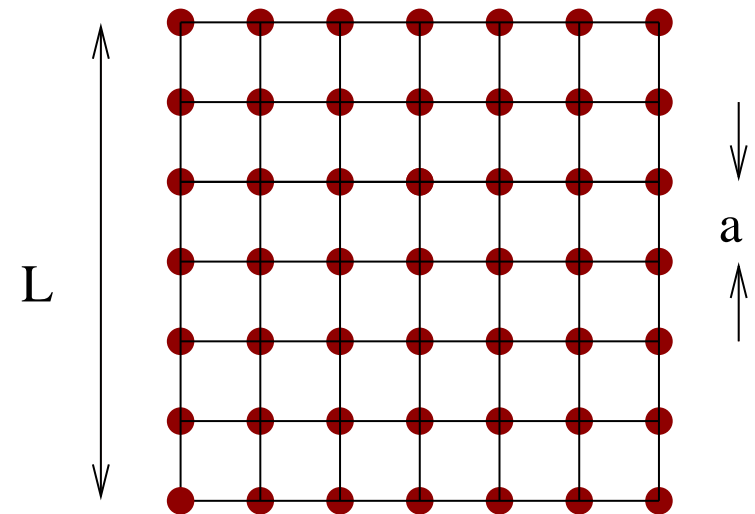
● In the continuum a judicious combination of WIs associated with translational invariance

$$\partial_\mu \langle T_{\mu\nu}(x)\, O_1 \ldots O_n \rangle = -\sum_{i=1}^{n} \langle O_1 \ldots \delta_x O_i \ldots O_n \rangle \ ,$$

leads to $(x_0 \neq y_0 \, , \, w_k \neq z_k)$

$$L_0 \, \langle \overline{T}_{0k}(x_0)\, T_{0k}(y) \rangle - L_k \, \langle \widetilde{T}_{0k}(w_k)\, T_{0k}(z) \rangle = \langle T_{00} \rangle - \langle T_{kk} \rangle$$

where

$$\overline{T}_{0k}(x_0) = \int d^3x \, T_{0k}(x) \ , \qquad \widetilde{T}_{0k}(x_k) = \int \Big[\prod_{\nu \neq k} dx_\nu \Big] T_{0k}(x)$$

● Note that:
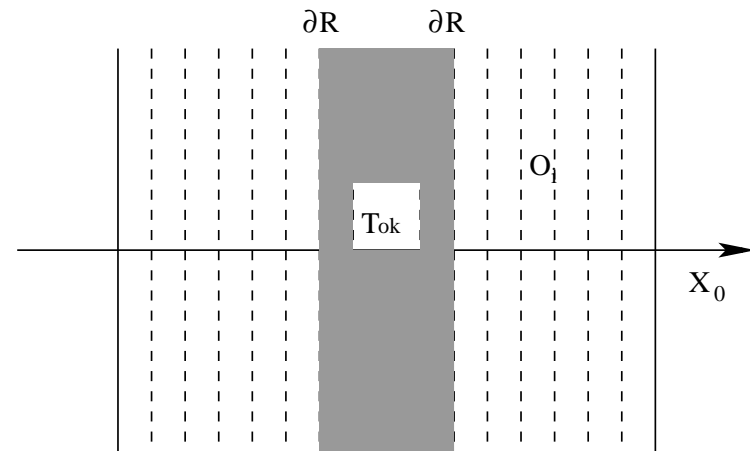
       ∗ All operators at non-zero distance

       ∗ Number of EMT on the two sides different

       ∗ Trace component of EMT does not contribute

       ∗ On the lattice it can be imposed to fix the renormalization of T_{0k}

Ward identities for two-point correlators of $\overline{T}_{0k}$ (II)

- The commutator of boost with momentum

$$[\hat{K}_k, \hat{p}_k] = i\hat{H}$$

is expressed in the Euclidean by the WIs

$$\int_{\partial R} d\sigma_\mu(x) \langle K_{\mu;0k}(x) \overline{T}_{0k}(y_0) O_1 \dots O_n \rangle_c = \langle \overline{T}_{00}(y_0) O_1 \dots O_n \rangle_c$$

when the O_i are localized external fields.

- In a 4D box boost transformations are incompatible with (periodic) boundary conditions. WIs associated with $SO(4)$ rotations must be modified by finite-size contributions

- The finite-volume theory is translational invariant, and it has a conserved $T_{\mu\nu}$. Modified WIs associated to boosts constructed from those associated to translational invariance

$$L_0 \langle \overline{T}_{0k}(x_0) T_{0k}(y) \rangle - L_k \langle \widetilde{T}_{0k}(w_k) T_{0k}(z) \rangle = \langle T_{00} \rangle - \langle T_{kk} \rangle$$

Ward identities for two-point correlators of $\overline{T}_{0k}$ (III)

- In the thermodynamic limit the WI reads ($y_0 \neq x_0$)

$$L_0 \langle \overline{T}_{0k}(x_0) \, T_{0k}(y) \rangle = \langle T_{00} \rangle - \langle T_{kk} \rangle$$

- By remembering that in the Euclidean

$$\hat{p}_k \leftrightarrow -i \, \overline{T}_{0k} \,, \quad e = -\langle T_{00} \rangle \,, \quad p = \langle T_{kk} \rangle \qquad \Longrightarrow \qquad \frac{\langle \hat{p}_k^2 \rangle}{V} = T \{ e + p \} = T^2 s$$

- In a finite box and for $M \neq 0$ (M lightest screening mass)

$$\langle \overline{T}_{0k}(x_0) \, T_{0k}(y) \rangle = -T \{ e + p \} + \frac{\nu M T^2}{2\pi L} \left[M + 3T \frac{\partial M}{\partial T} \right] e^{-ML} + \dots$$

i.e. leading finite-size effects are known functions of M, and are exponentially small in ML

Entropy density from shifted boundary conditions

- By putting together the two formulas

$$s = -\frac{1}{T^2} \lim_{V \to \infty} \frac{1}{V} \frac{d^2}{dz^2} \ln Z(\{0, 0, z\}) \Big|_{z=0}$$

- On the lattice the only difference is the discrete derivative

$$s = -\frac{1}{T^2} \lim_{V \to \infty} \lim_{a \to 0} \frac{2}{n_z^2 a^2 V} \ln \left[\frac{\mathcal{Z}(\{0, 0, n_z a\})}{\mathcal{Z}} \right]$$

with n_z being kept fixed when $a \to 0$

- Note that:

  * No ultraviolet renormalization

  * Finite volume effects exponentially small

  * Discretization effects $\mathcal{O}(a^2)$ once action improved

Recursive relation for higher order cumulants

- There is more information in $K(\mathbf{z})$. Again a judicious combination of WIs leads to

$$\langle \overline{T}_{0k}(x_0^1)\,\overline{T}_{0k}(x_0^2)\ldots\overline{T}_{0k}(x_0^{2n})\rangle_c = \langle \overline{T}_{00}(x_0^1)\,\overline{T}_{kk}(x_0^2)\ldots\overline{T}_{0k}(x_0^{2n})\rangle_c + \text{f.s.c.}$$

- At finite temperature and volume

$$L_0\,\langle \overline{T}_{00}(y_0)\,\overline{T}_{0k}(x_0^1)\ldots\overline{T}_{0k}(x_0^{2n})\rangle_c \;\; = \;\; L_0\,\frac{\partial}{\partial L_0}\,\langle \overline{T}_{0k}(x_0^1)\ldots\overline{T}_{0k}(x_0^{2n})\rangle_c$$

$$L_0\,\langle \overline{T}_{kk}(y_0)\,\overline{T}_{0k}(x_0^1)\ldots\overline{T}_{0k}(x_0^{2n})\rangle_c \;\; = \;\; \left\{L_k\,\frac{\partial}{\partial L_k} + 2n\right\}\langle \overline{T}_{0k}(x_0^1)\ldots\overline{T}_{0k}(x_0^{2n})\rangle_c$$

- By combining these relations, and by taking the infinite volume limit

$$\langle \overline{T}_{0k}(x_0^1)\ldots\overline{T}_{0k}(x_0^{2n})\rangle_c = (2n-1)\,\frac{\partial}{\partial L_0}\left\{\frac{1}{L_0}\,\langle \overline{T}_{0k}(x_0^1)\ldots\overline{T}_{0k}(x_0^{2n-2})\rangle_c\right\}$$

- Expression of finite-size corrections similar to the one of two-point corr. functions

Specific heat

- Written for cumulants the recursive relation reads

$$\langle \hat{p}_z^{2n} \rangle_c = (2n - 1)\, T^2\, \frac{\partial}{\partial T} \left\{ T\, \langle \hat{p}_z^{2n-2} \rangle_c \right\}$$

and analogously for mixed ones

- The definition of the specific heat implies

$$c_v = T \frac{\partial}{\partial T} s \qquad \Longrightarrow \qquad c_v = \frac{1}{V} \left[\frac{\langle \hat{p}_z^4 \rangle_c}{3 T^4} - 3\, \frac{\langle \hat{p}_z^2 \rangle_c}{T^2} \right]$$

and therefore

$$c_v = \lim_{V \to \infty} \frac{1}{V} \left[\frac{1}{3 T^4} \frac{d^4}{dz^4} + \frac{3}{T^2} \frac{d^2}{dz^2} \right] \ln Z(\{0, 0, z\}) \Big|_{z=0}$$

- On the lattice the only difference are the discrete derivatives. Finite-size corrections are again known, and are exponentially suppressed

Scale-invariant case

- If T is the only dimensionful parameter in the problem, the recursive relation implies

$$\frac{\langle \hat{p}_z^{2n} \rangle_c}{V} = c_{2n}\, T^{2n+3} \qquad \Longrightarrow \qquad c_{2n} = \frac{(n+1)}{4}\,(2n!)\,c_2$$

- By using the moment-cumulant transformation, the generator of the cumulants reads

$$K(\{0,0,z\}) = \sum_{n=1}^{\infty} (-1)^{n+1}\, \frac{\langle \hat{p}_z^{2n} \rangle_c}{2n!}\, z^{2n}$$

- The series can be re-summed to obtain

$$\frac{K(\{0,0,z\})}{V} = \frac{s}{4}\left\{ 1 - \frac{1}{(1+z^2 T^2)^2} \right\}$$

i.e. the entropy determines all the cumulants. The combination of scale and relativistic invariance fixes the functional form to be the one of the free case.

Numerical algorithm for the cumulant generator (I)

- The most straightforward way for computing
  the cumulant generator is to rewrite it as

$$\frac{\mathcal{Z}(\mathbf{z})}{\mathcal{Z}} = \prod_{i=0}^{n-1} \frac{\mathcal{Z}(\mathbf{z}, r_i)}{\mathcal{Z}(\mathbf{z}, r_{i+1})}$$

where a set of $(n + 1)$ systems is designed so
that the relevant phase spaces of successive path
integrals overlap and that $\mathcal{Z}(\mathbf{z}, r_0) = \mathcal{Z}(\mathbf{z})$ and
$\mathcal{Z}(\mathbf{z}, r_n) = \mathcal{Z}$
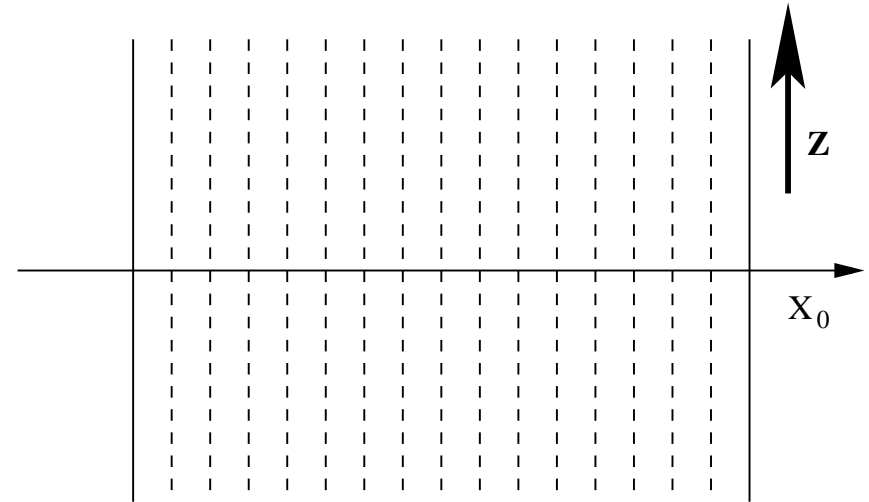
- The path integrals of the interpolating systems are defined as

$$\mathcal{Z}(\mathbf{z}, r) = \int DU \, DU_{4, L_0/a-1} \, e^{-\overline{S}_G[U, U_4, r]}$$

where $U_{4, L_0/a-1}$ is an extra (5th) temporal link assigned to each point of last time-slice

- The action of the interpolating systems is

$$\overline{S}_G[U, U_4, r] = S_G[U] + \frac{\beta}{3}(1 - r) \sum_{\mathbf{x}, k} \mathrm{ReTr}\Big\{ U_{0k}(L_0/a - 1, \mathbf{x}) - U_{4k}(L_0/a - 1, \mathbf{x}) \Big\}$$

  with the extra space-time plaquette given by

$$U_{4k}(L_0/a - 1, \mathbf{x}) = U_4(L_0/a - 1, \mathbf{x}) \, U_k(0, \mathbf{x} + \mathbf{z}) \, U_4^\dagger(L_0/a - 1, \mathbf{x} + \hat{k}) \, U_k^\dagger(L_0/a - 1, \mathbf{x})$$

- If we define the "reweighting" observable as

$$O[U, r_{i+1}] = e^{\overline{S}_G[U, U_4, r_{i+1}] - \overline{S}_G[U, U_4, r_i]}$$

  then

$$\frac{\mathcal{Z}(\mathbf{z}, r_i)}{\mathcal{Z}(\mathbf{z}, r_{i+1})} = \langle\, O[U, r_{i+1}]\, \rangle_{r_{i+1}}$$

- The action of the interpolating systems is

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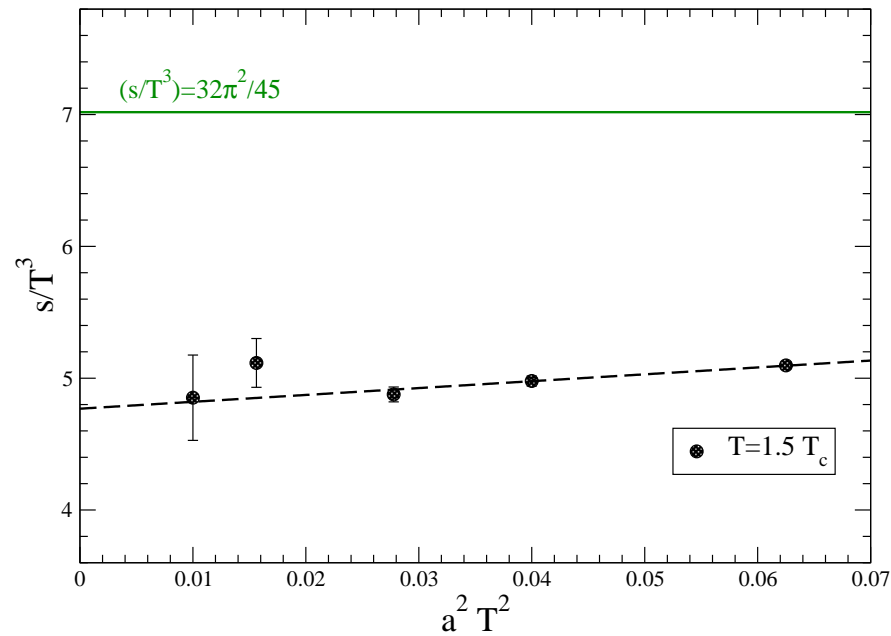
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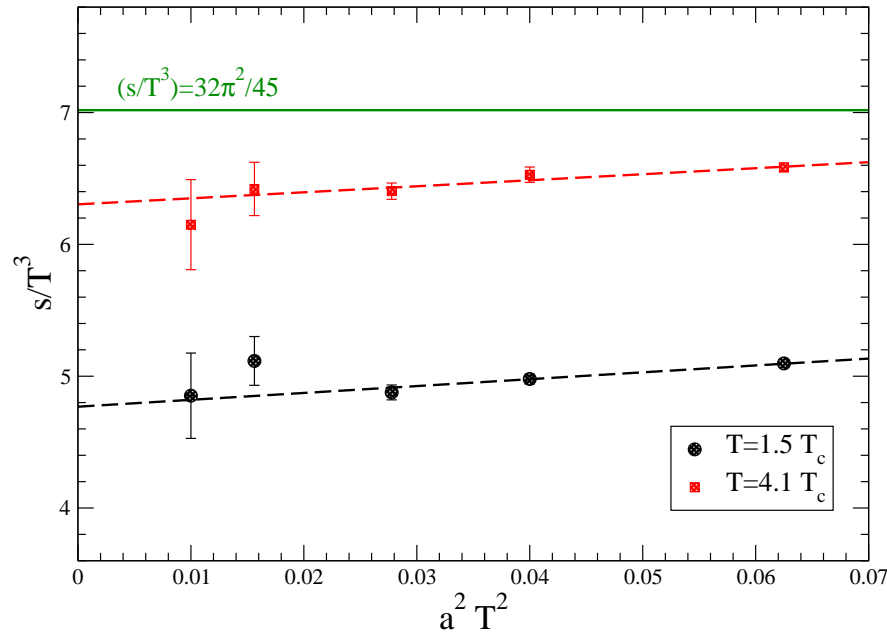- On each lattice the entropy is finally given by

$$s = -\frac{2}{\mathbf{z}^2 T^2 V} \sum_{i=0}^{n-1} \ln\left[\frac{\mathcal{Z}(\mathbf{z}, r_i)}{\mathcal{Z}(\mathbf{z}, r_{i+1})} \right]$$

Numerical results for the entropy

Lat	$6/g_0^2$	L_0/a	L/a	$K(\mathbf{z},a)$	$\dfrac{2K(\mathbf{z},a)}{|\mathbf{z}|^2 T^5 V}$
A_1	5.9	4	12	17.20(11)	5.10(3)
A_{1a}	5.9	4	16	40.71(15)	5.089(19)
A_2	6.024	5	16	13.05(10)	4.98(4)
A_3	6.137	6	18	7.32(8)	4.88(6)
A_4	6.337	8	24	4.32(16)	5.12(19)
A_5	6.507	10	30	2.62(17)	4.9(3)

Numerical results for the entropy

- A linear extrapolation in a^2 gives

$$\frac{s}{T^3} = 4.77 \pm 0.08 \pm ?? \qquad T = 1.5\,T_c$$

$$\frac{s}{T^3} = 6.30 \pm 0.09 \pm ?? \qquad T = 4.1\,T_c$$

- Compatible with previous computations, but continuum extrapolation must be improved

[Boyd et al. 96; Namekawa et al. 01]

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Lat	$6/g_0^2$	L_0/a	L/a	$K(\mathbf{z},a)$	$\frac{2K(\mathbf{z},a)}{|\mathbf{z}|^2 T^5 V}$
B_1	6.572	4	12	22.22(11)	6.58(3)
B_{1a}	6.572	4	16	53.47(16)	6.684(20)
B_2	6.747	5	16	17.11(15)	6.53(6)
B_3	6.883	6	18	9.61(9)	6.40(6)
B_4	7.135	8	24	5.42(17)	6.42(20)
B_5	7.325	10	30	3.32(18)	6.1(3)

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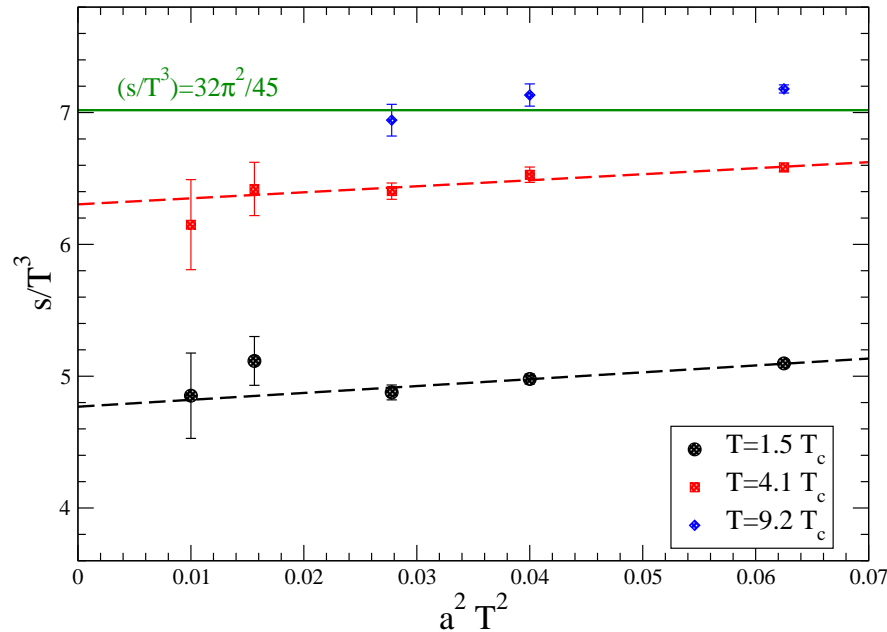
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Lat	$6/g_0^2$	L_0/a	L/a	$K(\mathbf{z},a)$	$\frac{2K(\mathbf{z},a)}{|\mathbf{z}|^2 T^5 V^3}$
C_1	7.234	4	16	57.44(25)	7.18(3)
C_2	7.426	5	20	36.5(4)	7.13(8)
C_3	7.584	6	24	24.7(4)	6.94(12)

Conclusions and outlook

- Correlation functions of total momentum fields can be related to derivatives of path integrals with shifted boundary conditions

- One of the applications is the computation of thermodynamic potentials, which can be connected to the cumulants via Ward identities of EMT. The entropy, for instance, is

$$s = -\frac{1}{T^2} \lim_{V \to \infty} \frac{1}{V} \frac{d^2}{dz^2} \ln Z(\{0, 0, z\})\Big|_{z=0}$$

- If lightest screening mass $M \neq 0$, leading finite-size corrections exponentially small in ML

- On the lattice these formulas apply once the derivative is discretized and the continuum limit is taken. No additive (vac. subtraction) or multiplicative UV renormalization is needed

- Same WIs allow for a non-perturbative renormalization of T_{0k}

- Feasibility study very promising even with a very simple-minded (expensive) algorithm